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A Particle-In-Cell Method for Modeling Small Angle Coulomb Collisions in Plasmas

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1 Introduction

We propose a computational method to self-consistently model small angle collisional effects. This method may be added to standard Particle-In-Cell (PIC) plasma simulations to include collisions, or as an alternative to solving the Fokker-Planck (FP) equation using finite difference methods. The distribution function is represented by a large number of particles. The particle velocities change due to the drag force, and the diffusion in velocity is represented by a random process. This is similar to previous Monte-Carlo methods [1,2], except we calculate the drag force and diffusion tensor self-consistently. The particles are weighted to a grid in velocity space and the associated "Poisson equations" are solved for the Rosenbluth potentials. The motivation is to avoid the very time consuming method of Coulomb scattering pair by pair. First the approximation for small angle Coulomb collisions is discussed. Next, the FP-PIC collision method is outlined. Then we show a test of the particle advance modeling an electron beam scattering off a fixed ion background.

2 Small angle Coulomb collisions

The FP equation for describing small angle Coulomb collisions can be solved numerically using finite difference techniques. An alternate method is to follow the evolution of a large number of particles. Using the notation of Trubnikov [3], an infinitestimal "cloud" of test particles can be represented by the quantities $< \Delta v_i >$ and $< \Delta v_i \Delta v_j >$ to the same order of accuracy as the FP equation[4], and are defined by:

$$< \Delta v_i > \equiv \frac{d\bar{v}_i(t)}{dt} \tag{1}$$

$$< \Delta v_i \Delta v_j > \equiv \frac{d}{dt}\left\{\overline{(v_i - \bar{v}_i)(v_j - \bar{v}_j)}\right\} \tag{2}$$

The bars represent averages. These may be interpreted as ensemble averages over many initial states, or as an ordinary average by letting the number of particles in a cloud, N, become large. We follow the second interpretation allowing a simpler simulation method.

$\bar{v}_i$ is now the average velocity of the local cloud. The i and j subscripts are the 3 velocity components in Cartesian coordinates, $(v_1 = v_x, v_2 = v_y, v_3 = v_z)$. $< \Delta v_i >$ is the drag force felt by an average particle in the cloud. $< \Delta v_i \Delta v_j >$ is the spreading or diffusion in velocity space of the cloud.

Numerically we advance the velocity of the particles by using the following equation [4]:

$$\Delta v_i(t^n) =< \Delta v_i > \Delta t + B_{ij} \Delta W_i(t^n) \tag{3}$$

where B_{ij} satisfies,

$$B_{ik} B_{kj} =< \Delta v_i \Delta v_j > \tag{4}$$

where $\Delta W_i(t^n) \equiv W_i(t^n) - W_i(t^{n-1})$, and $W_i(t)$ is a vector function that represents a Wiener process (or Brownian motion) having the following properties $< W_i(t) >= 0$ and $< W_i(t) W_j(t) >= t\delta_{ij}$. B and W are not unique and only need to satisfy the above criteria. In our model we choose:

$$\Delta W_i(t^n) = \sqrt{\Delta t} R_i \tag{5}$$

where R_i are independent random numbers satisfying $< R_i >= 0$, and $< R_i R_j >= \delta_{ij}$. We have found a a matrix B such that $BB^T = A$, given by:

$$B_{ij} = \begin{pmatrix} \sqrt{A_{11}} & 0 & 0 \\ \frac{A_{12}}{\sqrt{A_{11}}} & \sqrt{A_{22} - \frac{A_{12}^2}{A_{11}}} & 0 \\ \frac{A_{13}}{\sqrt{A_{11}}} & \frac{A_{23}}{B_{22}} - \frac{A_{12} A_{13}}{A_{11} B_{22}} & \sqrt{A_{33} - \frac{A_{13}^2}{A_{11}} - B_{32}^2} \end{pmatrix} \tag{6}$$

By letting $A_{ij} =< \Delta v_i \Delta v_j >$, we note that Eq. (6) satisfies Eq. (4) and can therefore use this B in Eq. (3).

The "field" quantities are obtained from two functions ϕ and ψ, the Rosenbluth potentials, which in turn are solved by the two Poisson equations [3]:

$$\nabla^2 \varphi^\beta = f^\beta(v_i) \tag{7}$$

$$\nabla^2 \psi^\beta = \phi^\beta(v_i) \tag{8}$$

where β is the superscript representing the field species, $\beta = (i, e)$. Then $< \Delta v_i >$ and $< \Delta v_i \Delta v_j >$ are obtained in terms of the Rosenbluth potentials using the following equation (see reference [3] for a derivation):

$$< \Delta v_i >^\alpha = - \sum_\beta \left(1 + \frac{m_\alpha}{m_\beta} \right) L^{\alpha/\beta} \frac{\partial \phi_\beta}{\partial v_i} \tag{9}$$

$$< \Delta v_i \Delta v_j >^{\alpha} = -2 \sum_{\beta} L^{\alpha/\beta} \frac{\partial^2 \psi_\beta}{\partial v_i \partial v_j} \tag{10}$$

$L^{\alpha/\beta} = \lambda \left(\frac{4\pi e_\alpha e_\beta}{m_\alpha} \right)^2$ is a constant (given here in cgs units), and λ is the Coulomb logarithm. α and β represent the test and field particles, respectively (e.g. $\alpha = (i,e)$ and $\beta = (i,e)$).

3 Outline of the Method

For the particle advance, we start with the simplest scheme [1], similar to Euler's method, except there is an added diffusion term (the last term on the right):

$$v_i^{n+1} = v_i^n + < \Delta v_i >^n \Delta t + B_{ij}^n \sqrt{\Delta t} R_j \tag{11}$$

R_j are independent random numbers having the two properties given above. Following a methodology similar to PIC simulation, we weight the particles to a grid, calculate the field quantities, advance the particles and repeat the process. The basic algorithm is as follows:

Step 1. Weight the particles to a grid in velocity space using linear interpolation.

Step 2. Solve Eqs. (7) and (8) on the grid for ϕ and ψ.

Step 3. Obtain $< \Delta v_i >^n$ and B_{ij}^n on the grid using Eqs. (6), (9) and (10).

Step 4. For each particle, obtain $< \Delta v_i >^n$ and B_{ij}^n by interpolating from the grid to the particle location v_i. Then, update the velocity using Eq. (11).

4 Test of the particle advance

As an initial test of the particle advance, Eq. (11), we model an electron beam scattered by infinitely massive cold ions. For this test case $< \Delta v_i >$ and $< \Delta v_i \Delta v_j >$ are given by the two simple analytic expressions:

$$< \Delta v_i > = -C \frac{v_i}{v^3} \tag{12}$$

$$< \Delta v_i \Delta v_j > = C \left(\frac{\delta_{ij}}{v} - \frac{v_i v_j}{v^3} \right) \tag{13}$$

where $C = \frac{n_\beta L^{\alpha/\beta}}{4\pi}$. We do not calculate the field quantities on the grid (step 1 and 2 above), but rather, use Eqs. (12) and (13) directly. This provides a good test of the particle advance, Eq. (11). We expect the total x-momentum to be given by [3]:

$$p_{x,total}(t) = p_{x,total}(t=0) exp\left(\frac{-C}{v_0^3} t \right) \tag{14}$$

where v_0 is the initial beam velocity. We have made a test run with the following parameters: $C = 1$, $v_0 = 1$, $v_{Te} = 0.01$ and $\Delta t = 0.001$. The energy error is less than 0.2 percent and the momentum error is less then 1 percent for a total time: T=1.

5 Future Work

We are developing a code to test the FP-PIC method outlined above. In the near future we plan to implement the algorithm in a 1d 3v electrostatic code in order to study combined collective electrostatic and collisional effects. With this code we would assume spatial homogeneity for calculating the collisional terms. If this assumption is not valid one would have to partition $f(v)$ into spatial regions j, and calculate $f_j(v)$ for each spatial region. One would have to ensure that enough particles in each spatial zone to adequately fill out the distribution function.

In addition, we need to address the accuracy and stability issues associated with this method, and study the feasibility of using a more accurate particle advancing scheme than that given by Eq. (11).

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